

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.09

Global applicability domain: Inside

Local applicability domain index: 5.23e-01

Confidence level: 6.34e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>O,O-Diethyl dithiophosphate</div> <div>Measured: 5.01</div> <div>Predicted: 5.43</div>	<div>Image not found</div> <div>Isophorone</div> <div>Measured: 2.00</div> <div>Predicted: 3.19</div>	<div>Image not found</div> <div>Triallylamine</div> <div>Measured: 3.55</div> <div>Predicted: 4.23</div>
<div>Image not found</div> <div>Thiram</div> <div>Measured: 3.39</div> <div>Predicted: 3.91</div>	<div>Image not found</div> <div>Menthol</div> <div>Measured: 10.8</div> <div>Predicted: 23.5</div>	<div>Image not found</div> <div>(1R,2S,5R)-(-)-Menthol</div> <div>Measured: 10.8</div> <div>Predicted: 23.5</div>